Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:30 pm BST

PDB ID	:	6FE7
Title	:	Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-356
Authors	:	Singh, A.K.; Brown, D.G.
Deposited on	:	2017-12-29
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

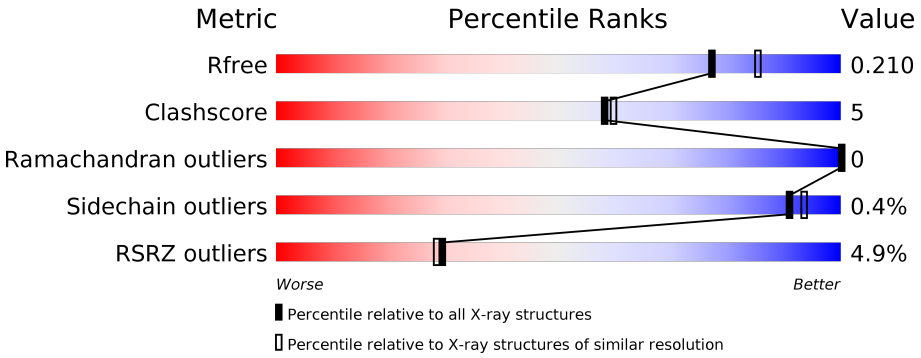
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	8% 84% 6% 9%
1	B	364	3% 85% • 11%
1	C	364	5% 80% 8% • 11%
1	D	364	2% 83% 6% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	512	-	-	-	X
4	EDO	D	522	-	X	-	-
8	PG4	C	521	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11789 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2669	1690	455	510	14			
1	B	323	Total	C	N	O	S	0	1	0
			2619	1657	447	501	14			
1	C	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	HIS	-	expression tag	UNP Q08499
A	78	MET	-	expression tag	UNP Q08499
B	75	GLY	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	HIS	-	expression tag	UNP Q08499
B	78	MET	-	expression tag	UNP Q08499
C	75	GLY	-	expression tag	UNP Q08499
C	76	SER	-	expression tag	UNP Q08499
C	77	HIS	-	expression tag	UNP Q08499
C	78	MET	-	expression tag	UNP Q08499
D	75	GLY	-	expression tag	UNP Q08499
D	76	SER	-	expression tag	UNP Q08499
D	77	HIS	-	expression tag	UNP Q08499
D	78	MET	-	expression tag	UNP Q08499

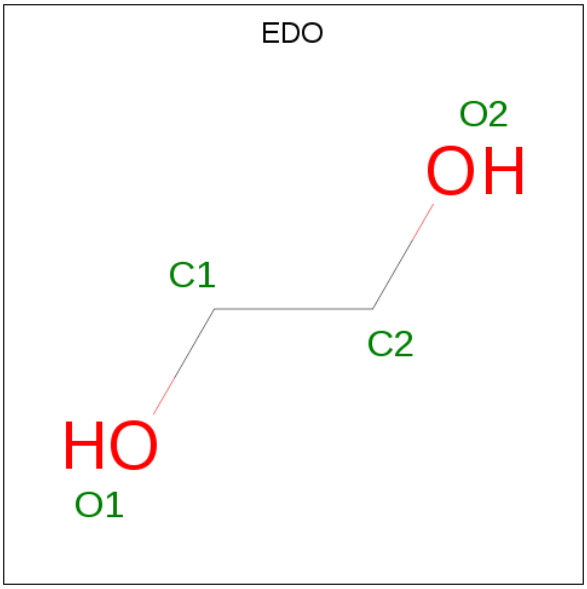
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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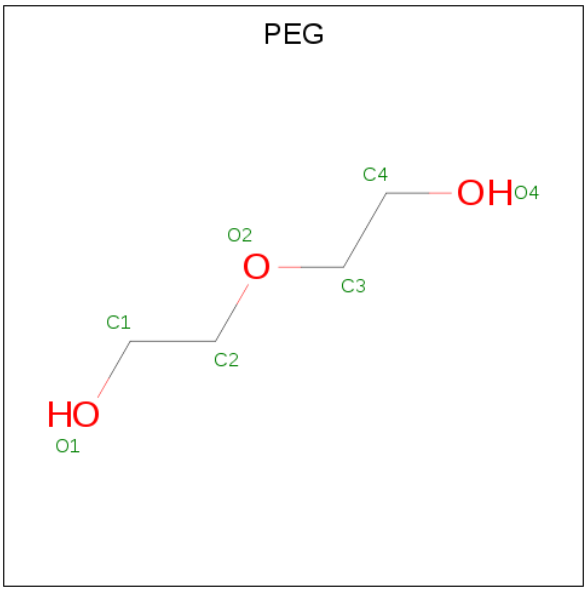
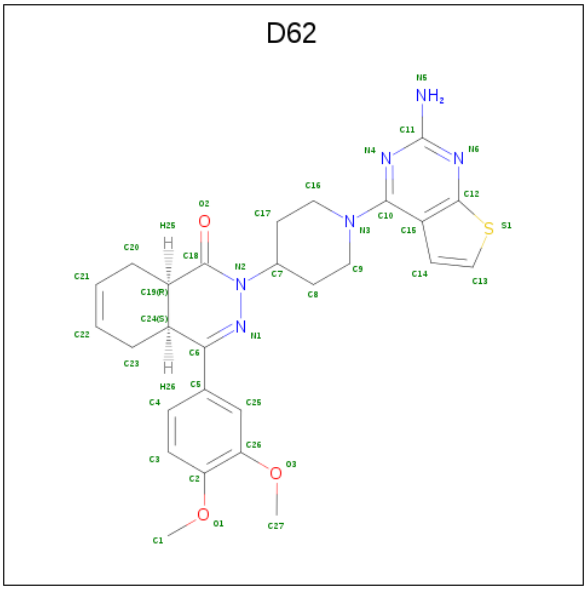
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



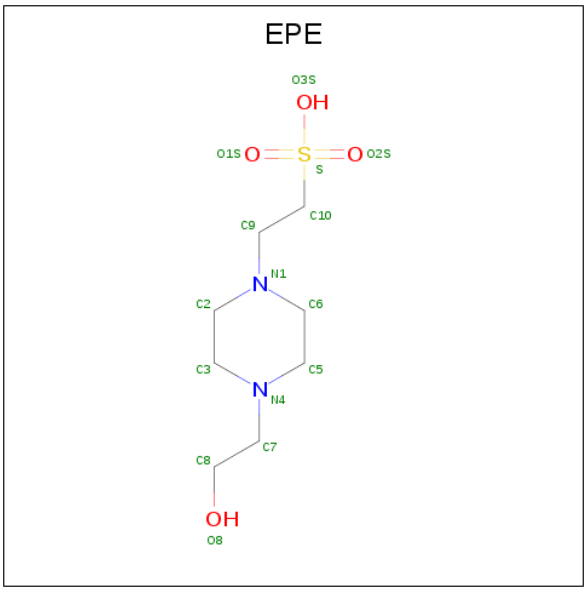
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0

- Molecule 6 is (4aS,8aR)-2-(1-{2-aminothieno[2,3-d]pyrimidin-4-yl}piperidin-4-yl)-4-(3,4- dimethoxyphenyl)-1,2,4a,5,8,8a-hexahydrophthalazin-1-one (three-letter code: D62) (formula: $C_{27}H_{30}N_6O_3S$).



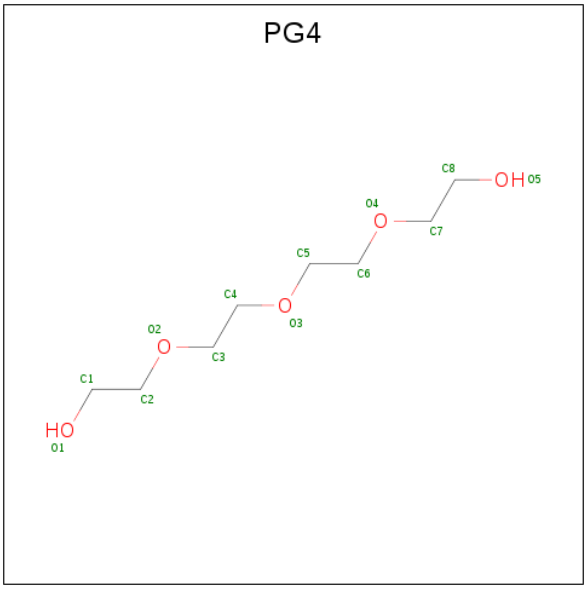
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	B	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	C	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	D	1	Total	C	N	O	S	0	0
			37	27	6	3	1		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 13 8 5	0	0
8	C	1	Total C O 13 8 5	0	0

- Molecule 9 is water.

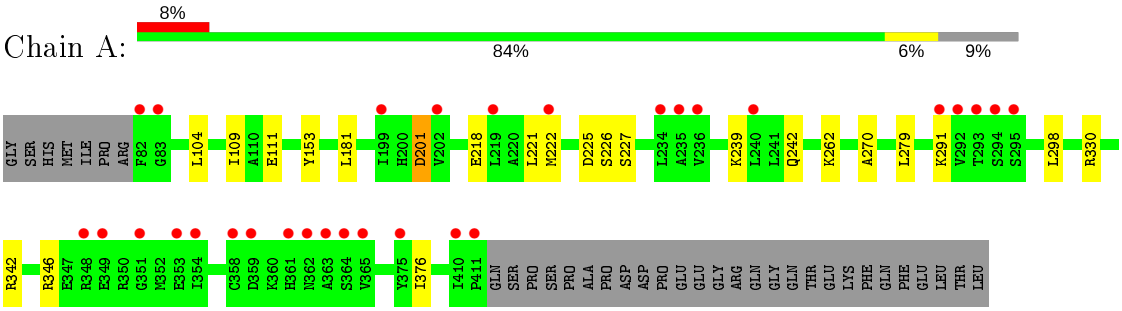
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	172	Total O 172 172	0	0
9	B	182	Total O 182 182	0	0
9	C	119	Total O 119 119	0	0
9	D	197	Total O 197 197	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

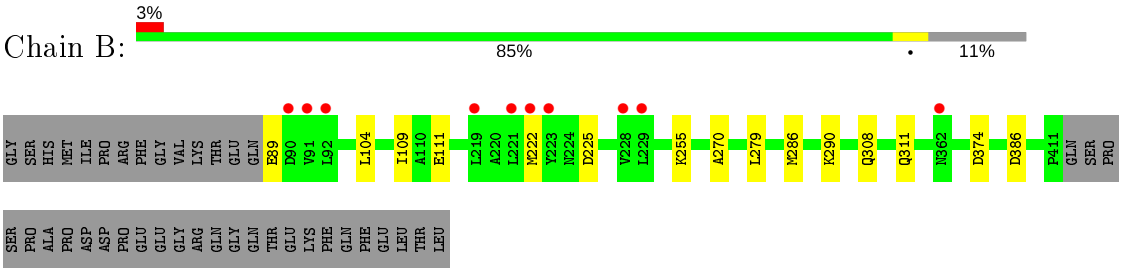
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



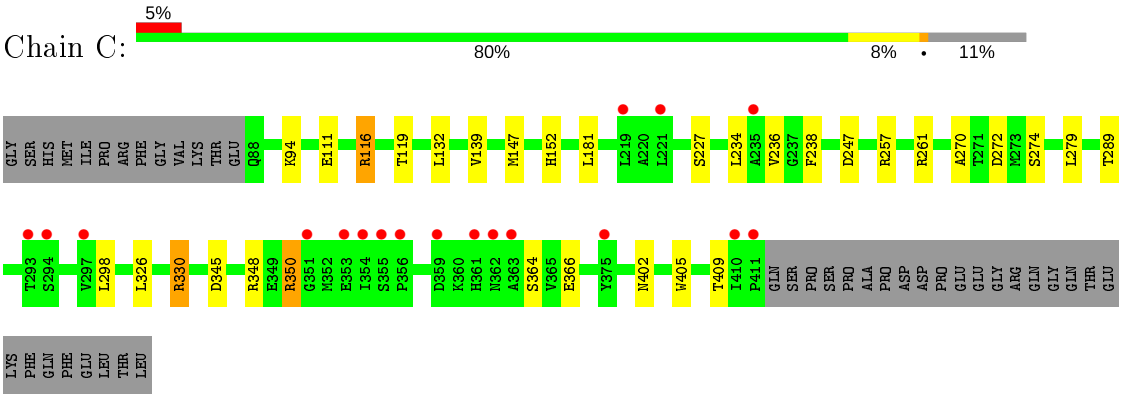
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



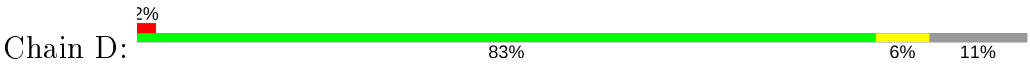
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

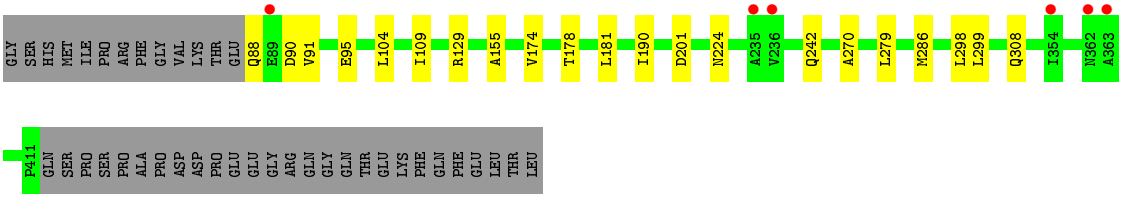
Chain C:



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain D:




GLY SER HIS MET ILE PRO ARG PHE GLY VAL LYS THR GLU
Q88 E89 D90 V91 E95 L104 I109 R129 A155 V174 T178 L181 I190 D201 N224 A235 V236 Q242 A270 L279 M286 L298 L299 Q308 I364 N362 A363
P411 GLN SER PRO SER PRO ALA PRO ASP ASP PRO GLU GLU GLY ARG GLN GLY GLN THR GLU LYS PHE GLN PHE GLU LEU THR LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.22Å 111.03Å 160.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.30 – 2.00 54.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.30-2.00) 100.0 (54.30-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.170 , 0.200 0.182 , 0.210	Depositor DCC
R_{free} test set	6067 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PEG, MG, EDO, PG4, EPE, D62

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.97	1/2724 (0.0%)	0.88	5/3700 (0.1%)
1	B	0.88	0/2673	0.83	0/3632
1	C	0.86	1/2676 (0.0%)	0.84	1/3636 (0.0%)
1	D	0.91	1/2676 (0.0%)	0.87	1/3636 (0.0%)
All	All	0.91	3/10749 (0.0%)	0.85	7/14604 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLU	CD-OE1	-5.47	1.19	1.25
1	D	95	GLU	CD-OE2	-5.13	1.20	1.25
1	C	364	SER	CB-OG	5.11	1.48	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ASP	CB-CG-OD2	12.36	129.42	118.30
1	A	201	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	A	330	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	C	350	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	330	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	D	201	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	225	ASP	CB-CG-OD1	5.63	123.37	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2669	0	2625	21	0
1	B	2619	0	2574	18	0
1	C	2622	0	2578	43	0
1	D	2622	0	2578	19	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	60	0	90	4	0
4	B	60	0	90	1	0
4	C	56	0	84	3	0
4	D	56	0	84	4	0
5	A	42	0	60	5	0
5	B	7	0	10	2	0
5	C	14	0	20	3	0
5	D	35	0	50	2	0
6	A	37	0	0	2	0
6	B	37	0	0	0	0
6	C	37	0	0	0	0
6	D	37	0	0	0	0
7	A	15	0	18	1	0
7	B	30	0	36	4	0
7	C	15	0	18	4	0
7	D	15	0	17	2	0
8	C	26	0	36	14	0
9	A	172	0	0	2	0
9	B	182	0	0	4	0
9	C	119	0	0	3	0
9	D	197	0	0	0	0
All	All	11789	0	10968	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLU:OE2	7:C:514:EPE:H32	1.65	0.95
1:B:111:GLU:OE1	7:B:521:EPE:H72	1.74	0.87
1:B:386:ASP:OD2	4:B:504:EDO:H22	1.75	0.87
1:C:116:ARG:HE	1:C:147:MET:CE	1.90	0.84
1:A:342:ARG:NH2	1:A:346:ARG:HH21	1.76	0.83
1:C:119:THR:OG1	1:C:147:MET:HE3	1.79	0.83
1:C:116:ARG:NE	1:C:147:MET:HE2	1.94	0.81
1:C:330:ARG:HG2	1:C:330:ARG:HH11	1.46	0.81
1:B:111:GLU:OE2	7:B:521:EPE:H52	1.82	0.80
8:C:521:PG4:H51	1:D:224:ASN:OD1	1.82	0.79
1:C:116:ARG:NE	1:C:147:MET:CE	2.47	0.78
1:D:129:ARG:HB3	4:D:521:EDO:H22	1.67	0.77
1:A:342:ARG:NH2	1:A:346:ARG:NH2	2.33	0.76
1:C:132:LEU:HD22	1:C:139:VAL:HG22	1.67	0.75
1:C:116:ARG:CZ	1:C:147:MET:HE2	2.19	0.72
8:C:521:PG4:H61	8:C:521:PG4:H31	1.71	0.72
1:D:286:MET:CE	1:D:308:GLN:OE1	2.38	0.72
1:D:88:GLN:HG3	1:D:90:ASP:H	1.56	0.70
1:C:330:ARG:HG2	1:C:330:ARG:NH1	2.04	0.69
1:A:201:ASP:OD2	2:A:501:ZN:ZN	1.42	0.68
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.27	0.67
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.11	0.67
1:C:261:ARG:HE	8:C:521:PG4:C8	2.07	0.66
1:C:330:ARG:CG	1:C:330:ARG:HH11	2.08	0.66
1:B:290:LYS:NZ	9:B:602:HOH:O	2.30	0.65
1:C:261:ARG:NE	8:C:521:PG4:H82	2.10	0.65
1:A:376:ILE:HD12	6:A:520:D62:C14	2.28	0.63
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.79	0.63
1:C:366:GLU:HG2	1:C:409:THR:OG1	1.99	0.63
1:C:132:LEU:CD2	1:C:139:VAL:HG22	2.28	0.63
5:A:518:PEG:H21	1:C:236:VAL:HG22	1.81	0.62
1:C:261:ARG:HE	8:C:521:PG4:H82	1.65	0.62
8:C:502:PG4:H41	9:C:698:HOH:O	2.00	0.61
1:C:111:GLU:OE2	7:C:514:EPE:H71	2.00	0.61
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.82	0.61
1:D:181:LEU:HD21	1:D:298:LEU:HD12	1.83	0.60
1:C:234:LEU:HB3	8:C:521:PG4:H52	1.82	0.60
7:D:523:EPE:H51	7:D:523:EPE:O8	2.03	0.58
9:A:603:HOH:O	1:C:350:ARG:NH2	2.37	0.58
1:D:88:GLN:HB3	1:D:91:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:525:EDO:H22	9:C:654:HOH:O	2.04	0.57
1:D:286:MET:HE3	1:D:308:GLN:OE1	2.04	0.57
1:A:227:SER:HA	5:A:516:PEG:H31	1.86	0.56
1:C:152:HIS:HE1	8:C:502:PG4:H52	1.71	0.56
1:D:190:ILE:HD13	4:D:521:EDO:H21	1.87	0.56
1:B:286:MET:CE	1:B:308:GLN:OE1	2.54	0.56
7:C:514:EPE:H92	9:C:705:HOH:O	2.06	0.56
1:C:116:ARG:NH1	1:C:147:MET:HE2	2.22	0.55
1:A:291:LYS:H	4:A:508:EDO:H11	1.70	0.55
1:C:326:LEU:HB2	4:C:515:EDO:H21	1.89	0.55
1:C:402:ASN:OD1	4:C:515:EDO:H12	2.08	0.54
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.89	0.54
1:D:174:VAL:HG12	5:D:519:PEG:H12	1.88	0.54
1:D:178:THR:OG1	5:D:519:PEG:H42	2.07	0.54
8:C:521:PG4:H61	8:C:521:PG4:C3	2.37	0.53
1:B:374:ASP:HA	5:B:508:PEG:H42	1.90	0.53
1:A:376:ILE:HD12	6:A:520:D62:C13	2.38	0.53
1:C:111:GLU:OE2	7:C:514:EPE:C3	2.49	0.53
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.91	0.52
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.39	0.52
1:C:261:ARG:HB2	4:C:509:EDO:H12	1.91	0.52
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.40	0.51
1:C:238:PHE:CD2	8:C:521:PG4:H72	2.46	0.51
1:B:111:GLU:CD	7:B:521:EPE:H52	2.30	0.51
1:C:227:SER:H	5:C:519:PEG:H32	1.76	0.51
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.41	0.50
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.93	0.50
1:A:153:TYR:O	4:A:525:EDO:H11	2.12	0.50
1:A:262:LYS:HG3	5:A:517:PEG:H32	1.93	0.49
5:A:517:PEG:H41	1:B:225:ASP:CB	2.42	0.49
1:A:222:MET:HE1	1:B:222:MET:HE3	1.94	0.49
1:B:255:LYS:HD3	9:B:693:HOH:O	2.12	0.49
1:C:116:ARG:HE	1:C:147:MET:HE1	1.73	0.49
1:C:405:TRP:O	1:C:409:THR:HG23	2.11	0.48
1:C:152:HIS:CE1	8:C:502:PG4:H52	2.49	0.48
1:C:261:ARG:NE	8:C:521:PG4:C8	2.73	0.48
1:D:286:MET:HE1	1:D:308:GLN:OE1	2.12	0.48
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.95	0.47
1:B:374:ASP:HA	5:B:508:PEG:C4	2.44	0.47
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.96	0.47
1:C:350:ARG:HD3	1:C:350:ARG:HH11	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.43	0.46
8:C:521:PG4:C6	8:C:521:PG4:C3	2.92	0.46
1:B:286:MET:HE3	1:B:308:GLN:OE1	2.15	0.46
1:C:272:ASP:OD2	5:C:519:PEG:H31	2.16	0.46
1:B:111:GLU:OE1	7:B:521:EPE:C7	2.54	0.45
1:A:342:ARG:CZ	1:A:346:ARG:NH2	2.79	0.45
1:D:181:LEU:CD2	1:D:298:LEU:HD12	2.46	0.45
1:C:152:HIS:HE1	8:C:502:PG4:C5	2.30	0.45
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.99	0.45
1:A:226:SER:HA	5:A:516:PEG:O1	2.17	0.44
1:C:289:THR:O	1:C:289:THR:HG22	2.17	0.44
1:D:129:ARG:CB	4:D:521:EDO:H22	2.43	0.44
1:B:311:GLN:OE1	9:B:601:HOH:O	2.21	0.43
1:A:239:LYS:HE3	1:A:242:GLN:OE1	2.18	0.43
4:A:521:EDO:O2	9:A:601:HOH:O	2.21	0.43
1:B:104:LEU:HD11	1:B:109:ILE:CD1	2.48	0.43
1:A:222:MET:HE3	1:B:222:MET:HE2	2.00	0.42
1:A:111:GLU:OE1	7:A:524:EPE:H52	2.20	0.41
1:C:116:ARG:NE	1:C:147:MET:HE1	2.29	0.41
1:C:274:SER:OG	5:C:519:PEG:H42	2.20	0.41
1:D:155:ALA:HA	4:D:513:EDO:H11	2.02	0.41
1:D:299:LEU:HD13	1:D:299:LEU:C	2.42	0.41
7:D:523:EPE:H102	7:D:523:EPE:H22	1.67	0.41
1:B:290:LYS:NZ	9:B:613:HOH:O	2.54	0.41
1:C:116:ARG:HA	1:C:116:ARG:HD2	1.87	0.41
1:C:247:ASP:OD2	1:C:257:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/364 (90%)	321 (98%)	7 (2%)	0	100	100
1	B	322/364 (88%)	317 (98%)	5 (2%)	0	100	100
1	C	322/364 (88%)	318 (99%)	4 (1%)	0	100	100
1	D	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
All	All	1294/1456 (89%)	1272 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/331 (91%)	300 (100%)	1 (0%)	92	95
1	B	296/331 (89%)	295 (100%)	1 (0%)	92	95
1	C	296/331 (89%)	293 (99%)	3 (1%)	76	81
1	D	296/331 (89%)	296 (100%)	0	100	100
All	All	1189/1324 (90%)	1184 (100%)	5 (0%)	91	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	B	89	GLU
1	C	94	LYS
1	C	116	ARG
1	C	330	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	308	GLN
1	B	231	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 91 ligands modelled in this entry, 8 are monoatomic - leaving 83 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	C	503	-	3,3,3	0.42	0	2,2,2	0.47	0
4	EDO	A	507	-	3,3,3	0.29	0	2,2,2	1.50	0
4	EDO	C	507	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.52	0
4	EDO	A	521	-	3,3,3	0.52	0	2,2,2	0.76	0
5	PEG	A	511	-	6,6,6	0.40	0	5,5,5	0.59	0
5	PEG	A	518	-	6,6,6	0.61	0	5,5,5	0.68	0
4	EDO	A	515	-	3,3,3	1.18	0	2,2,2	0.43	0
5	PEG	D	518	-	6,6,6	1.08	0	5,5,5	1.30	0
6	D62	C	520	-	40,42,42	0.74	2 (5%)	45,61,61	1.21	3 (6%)
4	EDO	D	505	-	3,3,3	0.49	0	2,2,2	0.45	0
4	EDO	A	509	-	3,3,3	0.54	0	2,2,2	0.37	0
4	EDO	C	512	-	3,3,3	0.96	0	2,2,2	0.69	0
5	PEG	B	508	-	6,6,6	0.77	0	5,5,5	1.39	1 (20%)
4	EDO	D	514	-	3,3,3	1.04	0	2,2,2	0.58	0
4	EDO	C	509	-	3,3,3	0.30	0	2,2,2	0.43	0
4	EDO	A	523	-	3,3,3	0.50	0	2,2,2	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	C	510	-	3,3,3	0.18	0	2,2,2	0.92	0
4	EDO	B	504	-	3,3,3	0.27	0	2,2,2	0.62	0
7	EPE	B	509	-	15,15,15	1.33	1 (6%)	18,20,20	2.44	7 (38%)
6	D62	D	517	-	40,42,42	0.83	1 (2%)	45,61,61	1.33	3 (6%)
4	EDO	A	514	-	3,3,3	0.53	0	2,2,2	0.78	0
5	PEG	A	510	-	6,6,6	0.51	0	5,5,5	0.73	0
7	EPE	B	521	-	15,15,15	2.04	1 (6%)	18,20,20	1.12	3 (16%)
4	EDO	D	520	-	3,3,3	0.32	0	2,2,2	0.90	0
4	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.38	0
6	D62	A	520	-	40,42,42	0.82	2 (5%)	45,61,61	1.17	5 (11%)
4	EDO	D	506	-	3,3,3	0.32	0	2,2,2	1.15	0
5	PEG	A	517	-	6,6,6	0.53	0	5,5,5	0.52	0
4	EDO	D	515	-	3,3,3	0.46	0	2,2,2	1.32	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	1.19	0
4	EDO	B	506	-	3,3,3	0.37	0	2,2,2	1.48	1 (50%)
4	EDO	D	521	-	3,3,3	0.61	0	2,2,2	0.88	0
4	EDO	C	501	-	3,3,3	0.54	0	2,2,2	0.19	0
4	EDO	B	507	-	3,3,3	0.29	0	2,2,2	1.55	0
8	PG4	C	502	-	12,12,12	1.03	0	11,11,11	1.01	0
4	EDO	D	507	-	3,3,3	0.46	0	2,2,2	0.46	0
5	PEG	A	516	-	6,6,6	0.72	0	5,5,5	1.15	0
4	EDO	A	512	-	3,3,3	0.31	0	2,2,2	1.23	0
5	PEG	C	519	-	6,6,6	0.91	0	5,5,5	1.22	0
4	EDO	A	504	-	3,3,3	0.40	0	2,2,2	0.92	0
4	EDO	D	504	-	3,3,3	0.77	0	2,2,2	0.21	0
5	PEG	A	519	-	6,6,6	0.43	0	5,5,5	0.45	0
4	EDO	D	512	-	3,3,3	0.47	0	2,2,2	0.23	0
5	PEG	D	509	-	6,6,6	0.98	0	5,5,5	1.64	1 (20%)
4	EDO	D	501	-	3,3,3	0.76	0	2,2,2	0.36	0
4	EDO	B	520	-	3,3,3	0.42	0	2,2,2	0.64	0
4	EDO	A	505	-	3,3,3	0.51	0	2,2,2	0.25	0
5	PEG	D	519	-	6,6,6	0.48	0	5,5,5	1.28	0
4	EDO	B	512	-	3,3,3	0.09	0	2,2,2	1.11	0
4	EDO	C	511	-	3,3,3	0.61	0	2,2,2	0.64	0
4	EDO	B	518	-	3,3,3	0.83	0	2,2,2	0.28	0
8	PG4	C	521	-	12,12,12	1.26	2 (16%)	11,11,11	1.58	2 (18%)
4	EDO	A	506	-	3,3,3	0.71	0	2,2,2	1.03	0
4	EDO	D	513	-	3,3,3	0.79	0	2,2,2	1.16	0
5	PEG	D	510	-	6,6,6	0.34	0	5,5,5	0.89	0
7	EPE	D	523	-	15,15,15	2.99	4 (26%)	18,20,20	1.82	6 (33%)
4	EDO	B	517	-	3,3,3	0.19	0	2,2,2	1.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	B	510	-	3,3,3	0.48	0	2,2,2	0.87	0
4	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.16	0
4	EDO	C	517	-	3,3,3	0.32	0	2,2,2	0.69	0
4	EDO	B	513	-	3,3,3	0.58	0	2,2,2	0.68	0
4	EDO	A	522	-	3,3,3	0.58	0	2,2,2	0.47	0
4	EDO	A	503	-	3,3,3	0.36	0	2,2,2	0.73	0
6	D62	B	516	-	40,42,42	0.76	1 (2%)	45,61,61	1.14	6 (13%)
4	EDO	A	525	-	3,3,3	0.77	0	2,2,2	0.11	0
4	EDO	C	522	-	3,3,3	0.45	0	2,2,2	0.47	0
7	EPE	C	514	-	15,15,15	2.03	1 (6%)	18,20,20	1.10	3 (16%)
4	EDO	C	515	-	3,3,3	0.86	0	2,2,2	0.34	0
4	EDO	D	511	-	3,3,3	0.47	0	2,2,2	0.86	0
4	EDO	C	508	-	3,3,3	0.47	0	2,2,2	0.62	0
4	EDO	B	514	-	3,3,3	0.77	0	2,2,2	0.29	0
4	EDO	B	511	-	3,3,3	0.69	0	2,2,2	1.20	0
4	EDO	C	516	-	3,3,3	1.03	0	2,2,2	0.88	0
7	EPE	A	524	-	15,15,15	2.38	1 (6%)	18,20,20	2.82	7 (38%)
4	EDO	B	515	-	3,3,3	0.36	0	2,2,2	0.53	0
4	EDO	C	518	-	3,3,3	0.29	0	2,2,2	0.69	0
5	PEG	C	513	-	6,6,6	0.52	0	5,5,5	0.94	0
4	EDO	A	513	-	3,3,3	0.27	0	2,2,2	1.50	1 (50%)
4	EDO	B	519	-	3,3,3	0.29	0	2,2,2	1.12	0
4	EDO	D	522	-	3,3,3	2.63	3 (100%)	2,2,2	2.36	2 (100%)
5	PEG	D	508	-	6,6,6	0.49	0	5,5,5	1.21	0
4	EDO	D	516	-	3,3,3	0.51	0	2,2,2	1.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	503	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	A	521	-	-	1/1/1/1	-
5	PEG	A	511	-	-	4/4/4/4	-
5	PEG	A	518	-	-	2/4/4/4	-
4	EDO	A	515	-	-	0/1/1/1	-
5	PEG	D	518	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D62	C	520	-	-	2/16/53/53	0/6/6/6
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	C	512	-	-	1/1/1/1	-
5	PEG	B	508	-	-	1/4/4/4	-
4	EDO	D	514	-	-	0/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
7	EPE	B	509	-	-	3/9/19/19	0/1/1/1
6	D62	D	517	-	-	2/16/53/53	0/6/6/6
4	EDO	A	514	-	-	1/1/1/1	-
5	PEG	A	510	-	-	3/4/4/4	-
7	EPE	B	521	-	-	2/9/19/19	0/1/1/1
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
6	D62	A	520	-	-	1/16/53/53	0/6/6/6
4	EDO	D	506	-	-	0/1/1/1	-
5	PEG	A	517	-	-	3/4/4/4	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
8	PG4	C	502	-	-	5/10/10/10	-
4	EDO	D	507	-	-	1/1/1/1	-
5	PEG	A	516	-	-	3/4/4/4	-
4	EDO	A	512	-	-	0/1/1/1	-
5	PEG	C	519	-	-	2/4/4/4	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
5	PEG	A	519	-	-	1/4/4/4	-
4	EDO	D	512	-	-	1/1/1/1	-
5	PEG	D	509	-	-	3/4/4/4	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	B	520	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
5	PEG	D	519	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	C	511	-	-	0/1/1/1	-
4	EDO	B	518	-	-	1/1/1/1	-
8	PG4	C	521	-	-	7/10/10/10	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
5	PEG	D	510	-	-	0/4/4/4	-
7	EPE	D	523	-	-	3/9/19/19	0/1/1/1
4	EDO	B	517	-	-	0/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
6	D62	B	516	-	-	2/16/53/53	0/6/6/6
4	EDO	A	525	-	-	0/1/1/1	-
4	EDO	C	522	-	-	0/1/1/1	-
7	EPE	C	514	-	-	6/9/19/19	0/1/1/1
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	D	511	-	-	1/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	B	514	-	-	0/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
7	EPE	A	524	-	-	3/9/19/19	0/1/1/1
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
5	PEG	C	513	-	-	3/4/4/4	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	D	522	-	-	0/1/1/1	-
5	PEG	D	508	-	-	3/4/4/4	-
4	EDO	D	516	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	523	EPE	C10-S	-10.83	1.62	1.77
7	A	524	EPE	C10-S	-8.72	1.65	1.77
7	C	514	EPE	C10-S	-7.66	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	521	EPE	C10-S	-7.66	1.66	1.77
7	B	509	EPE	C10-S	-4.18	1.71	1.77
4	D	522	EDO	O1-C1	3.25	1.58	1.42
6	D	517	D62	C10-N4	3.03	1.36	1.32
6	A	520	D62	C10-N4	2.77	1.36	1.32
6	B	516	D62	C10-N4	2.77	1.36	1.32
6	A	520	D62	C15-C12	-2.67	1.38	1.42
6	C	520	D62	C10-N4	2.50	1.35	1.32
4	D	522	EDO	O2-C2	2.49	1.54	1.42
6	C	520	D62	C15-C12	-2.44	1.38	1.42
8	C	521	PG4	C6-C5	2.28	1.60	1.49
7	D	523	EPE	O2S-S	-2.19	1.38	1.45
7	D	523	EPE	O3S-S	-2.15	1.40	1.47
8	C	521	PG4	O2-C3	2.14	1.51	1.42
7	D	523	EPE	O1S-S	-2.06	1.38	1.45
4	D	522	EDO	C2-C1	2.00	1.62	1.48

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	524	EPE	O3S-S-C10	7.35	117.65	105.77
7	A	524	EPE	O2S-S-C10	-6.90	98.60	106.92
7	B	509	EPE	O2S-S-C10	4.93	112.85	106.92
7	B	509	EPE	O1S-S-C10	4.90	112.81	106.92
6	D	517	D62	C8-C7-N2	-4.25	106.15	110.86
7	B	509	EPE	C5-N4-C3	4.24	118.38	108.83
6	C	520	D62	C8-C7-N2	-3.55	106.93	110.86
7	A	524	EPE	O3S-S-O2S	-3.54	102.62	111.27
6	D	517	D62	C4-C5-C6	3.30	124.66	120.75
7	D	523	EPE	O2S-S-O1S	-3.29	102.57	113.95
8	C	521	PG4	C3-O2-C2	3.24	127.32	113.29
7	A	524	EPE	O1S-S-C10	3.08	110.63	106.92
7	D	523	EPE	O2S-S-C10	3.06	110.60	106.92
5	D	509	PEG	C3-O2-C2	2.91	125.90	113.29
7	B	509	EPE	C2-C3-N4	2.89	116.58	110.64
6	D	517	D62	C13-S1-C12	-2.88	87.28	91.00
7	D	523	EPE	C3-C2-N1	-2.87	104.75	110.64
8	C	521	PG4	O2-C2-C1	2.87	122.68	110.07
6	A	520	D62	C8-C7-N2	-2.84	107.71	110.86
7	D	523	EPE	C5-C6-N1	-2.77	104.96	110.64
6	A	520	D62	N6-C11-N4	-2.75	123.55	127.22
6	C	520	D62	C13-S1-C12	-2.74	87.46	91.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	522	EDO	O1-C1-C2	2.66	131.02	111.91
7	D	523	EPE	O1S-S-C10	2.62	110.07	106.92
6	B	516	D62	C8-C7-N2	-2.55	108.04	110.86
7	B	509	EPE	C5-C6-N1	-2.52	105.47	110.64
6	B	516	D62	O2-C18-N2	-2.51	118.58	121.64
7	D	523	EPE	O3S-S-C10	2.41	109.67	105.77
6	B	516	D62	N6-C11-N4	-2.36	124.07	127.22
6	C	520	D62	N6-C11-N4	-2.31	124.14	127.22
7	C	514	EPE	O3S-S-C10	2.30	109.48	105.77
7	B	521	EPE	O3S-S-C10	2.29	109.47	105.77
6	B	516	D62	C11-N4-C10	2.25	120.14	113.91
7	B	509	EPE	O3S-S-O2S	-2.21	105.88	111.27
6	A	520	D62	C11-N4-C10	2.19	119.97	113.91
7	A	524	EPE	C5-N4-C3	2.17	113.72	108.83
6	A	520	D62	C15-C10-N4	-2.16	118.06	122.66
7	C	514	EPE	O1S-S-C10	2.16	109.52	106.92
7	B	509	EPE	O3S-S-C10	-2.16	102.27	105.77
7	B	521	EPE	O2S-S-C10	2.16	109.51	106.92
4	A	513	EDO	O1-C1-C2	-2.12	96.65	111.91
6	B	516	D62	O2-C18-C19	2.12	127.01	121.88
6	B	516	D62	C15-C10-N4	-2.11	118.17	122.66
5	B	508	PEG	O4-C4-C3	2.11	124.04	111.81
7	B	521	EPE	O1S-S-C10	2.11	109.45	106.92
7	A	524	EPE	C7-N4-C3	2.11	116.62	111.23
7	C	514	EPE	O2S-S-C10	2.10	109.45	106.92
7	A	524	EPE	C3-C2-N1	-2.09	106.34	110.64
4	B	506	EDO	O2-C2-C1	-2.09	96.87	111.91
6	A	520	D62	C4-C5-C6	2.09	123.22	120.75
4	D	522	EDO	O2-C2-C1	2.02	126.44	111.91

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	516	D62	N4-C10-N3-C9
4	D	507	EDO	O1-C1-C2-O2
7	C	514	EPE	C10-C9-N1-C6
7	C	514	EPE	S-C10-C9-N1
7	C	514	EPE	C9-C10-S-O2S
7	A	524	EPE	C8-C7-N4-C3
6	C	520	D62	C15-C10-N3-C9
6	C	520	D62	N4-C10-N3-C9

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Mol	Chain	Res	Type	Atoms
7	B	521	EPE	S-C10-C9-N1
7	D	523	EPE	C10-C9-N1-C2
7	D	523	EPE	C8-C7-N4-C5
7	D	523	EPE	C9-C10-S-O1S
6	D	517	D62	C15-C10-N3-C9
6	D	517	D62	N4-C10-N3-C9
7	B	509	EPE	C10-C9-N1-C6
6	A	520	D62	N4-C10-N3-C9
5	C	519	PEG	C4-C3-O2-C2
8	C	521	PG4	O2-C3-C4-O3
5	D	519	PEG	C1-C2-O2-C3
8	C	521	PG4	C1-C2-O2-C3
8	C	521	PG4	O3-C5-C6-O4
5	D	518	PEG	O1-C1-C2-O2
8	C	521	PG4	O1-C1-C2-O2
5	D	508	PEG	O2-C3-C4-O4
8	C	502	PG4	O1-C1-C2-O2
5	C	513	PEG	O1-C1-C2-O2
7	C	514	EPE	C9-C10-S-O3S
5	A	517	PEG	O2-C3-C4-O4
5	A	516	PEG	O1-C1-C2-O2
5	C	519	PEG	O2-C3-C4-O4
5	B	508	PEG	O1-C1-C2-O2
5	D	509	PEG	O1-C1-C2-O2
5	A	511	PEG	O2-C3-C4-O4
5	A	510	PEG	O2-C3-C4-O4
5	A	516	PEG	O2-C3-C4-O4
4	C	512	EDO	O1-C1-C2-O2
4	A	514	EDO	O1-C1-C2-O2
4	D	520	EDO	O1-C1-C2-O2
4	C	510	EDO	O1-C1-C2-O2
4	B	512	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	C	517	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
4	A	522	EDO	O1-C1-C2-O2
8	C	502	PG4	O3-C5-C6-O4
5	A	511	PEG	O1-C1-C2-O2
8	C	521	PG4	C6-C5-O3-C4
8	C	521	PG4	O4-C7-C8-O5
5	D	519	PEG	O2-C3-C4-O4
4	A	523	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	507	EDO	O1-C1-C2-O2
7	A	524	EPE	S-C10-C9-N1
7	B	509	EPE	C10-C9-N1-C2
5	A	511	PEG	C4-C3-O2-C2
4	C	508	EDO	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2
4	A	521	EDO	O1-C1-C2-O2
4	A	509	EDO	O1-C1-C2-O2
4	B	519	EDO	O1-C1-C2-O2
5	A	518	PEG	O2-C3-C4-O4
5	C	513	PEG	O2-C3-C4-O4
8	C	521	PG4	C5-C6-O4-C7
5	D	509	PEG	C4-C3-O2-C2
5	A	510	PEG	C1-C2-O2-C3
6	B	516	D62	C15-C10-N3-C9
5	A	518	PEG	C4-C3-O2-C2
5	D	519	PEG	O1-C1-C2-O2
5	A	517	PEG	C4-C3-O2-C2
5	A	517	PEG	C1-C2-O2-C3
5	D	508	PEG	O1-C1-C2-O2
7	C	514	EPE	C9-C10-S-O1S
5	A	510	PEG	C4-C3-O2-C2
5	D	508	PEG	C1-C2-O2-C3
4	B	518	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
7	B	521	EPE	N4-C7-C8-O8
8	C	502	PG4	C5-C6-O4-C7
5	D	509	PEG	O2-C3-C4-O4
8	C	502	PG4	C1-C2-O2-C3
4	D	512	EDO	O1-C1-C2-O2
4	B	520	EDO	O1-C1-C2-O2
4	D	511	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	C	518	EDO	O1-C1-C2-O2
5	A	511	PEG	C1-C2-O2-C3
5	A	516	PEG	C4-C3-O2-C2
7	C	514	EPE	N4-C7-C8-O8
4	B	505	EDO	O1-C1-C2-O2
4	D	521	EDO	O1-C1-C2-O2
4	C	501	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	504	EDO	O1-C1-C2-O2
4	D	501	EDO	O1-C1-C2-O2
5	A	519	PEG	O1-C1-C2-O2
8	C	502	PG4	O2-C3-C4-O3
4	C	503	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
7	A	524	EPE	C9-C10-S-O2S
7	B	509	EPE	C9-C10-S-O2S
5	C	513	PEG	C1-C2-O2-C3

There are no ring outliers.

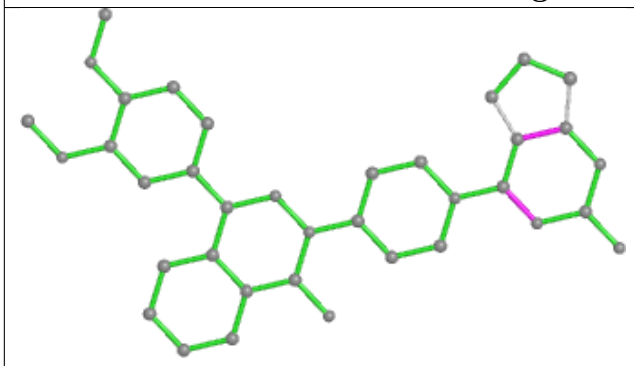
21 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	521	EDO	1	0
5	A	518	PEG	1	0
5	B	508	PEG	2	0
4	C	509	EDO	1	0
4	B	504	EDO	1	0
7	B	521	EPE	4	0
4	A	508	EDO	1	0
6	A	520	D62	2	0
5	A	517	PEG	2	0
4	D	521	EDO	3	0
8	C	502	PG4	4	0
5	A	516	PEG	2	0
5	C	519	PEG	3	0
5	D	519	PEG	2	0
8	C	521	PG4	10	0
4	D	513	EDO	1	0
7	D	523	EPE	2	0
4	A	525	EDO	2	0
7	C	514	EPE	4	0
4	C	515	EDO	2	0
7	A	524	EPE	1	0

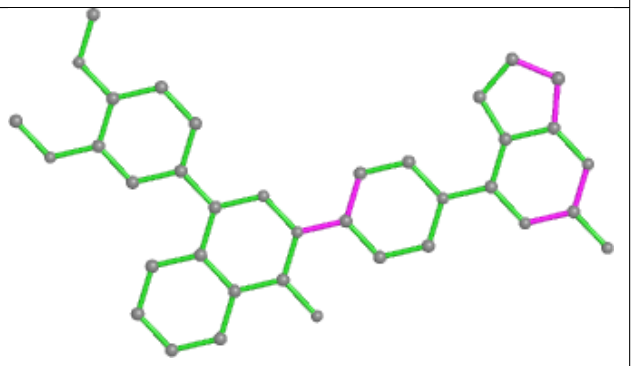
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

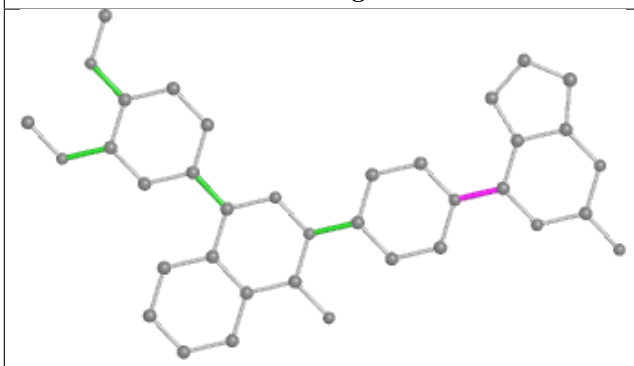
Ligand D62 C 520



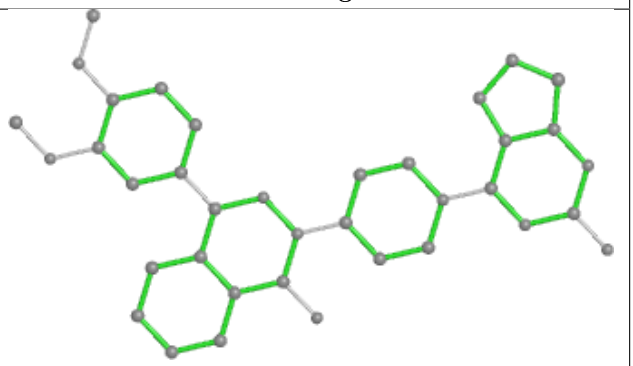
Bond lengths



Bond angles

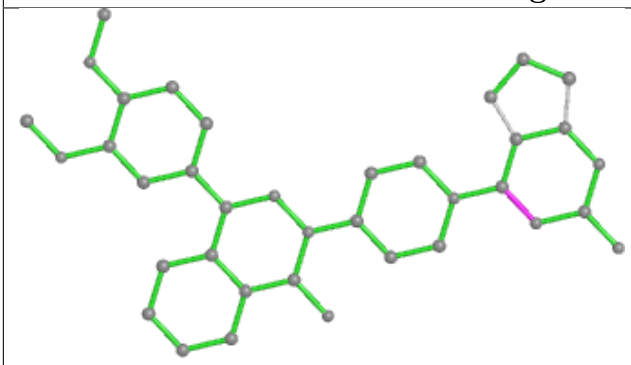


Torsions

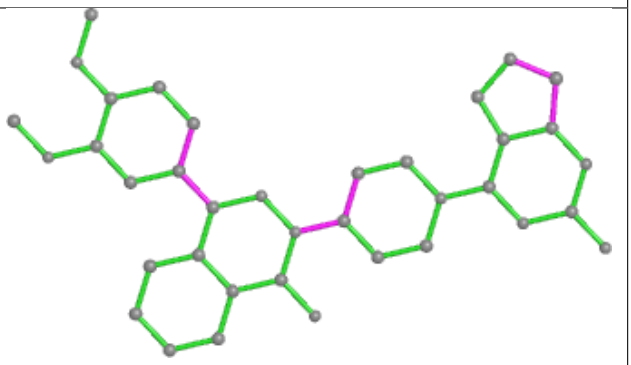


Rings

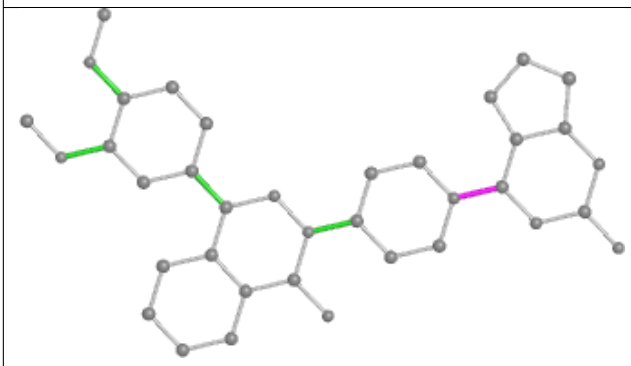
Ligand D62 D 517



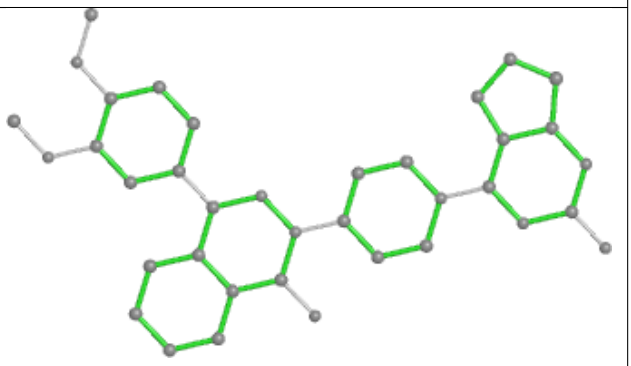
Bond lengths



Bond angles

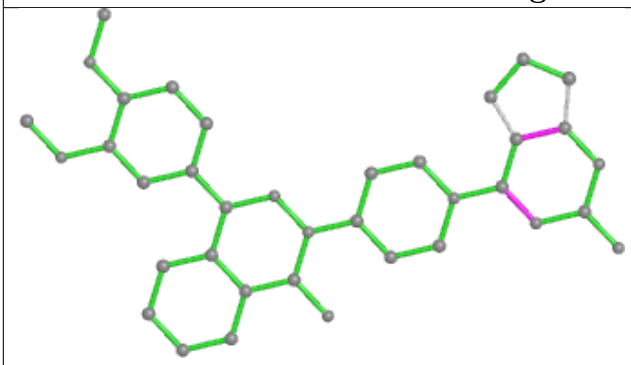


Torsions

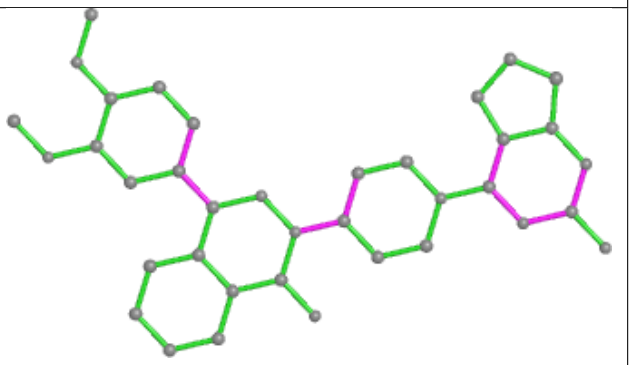


Rings

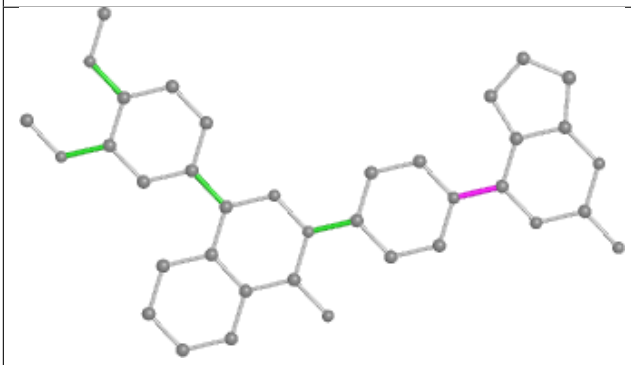
Ligand D62 A 520



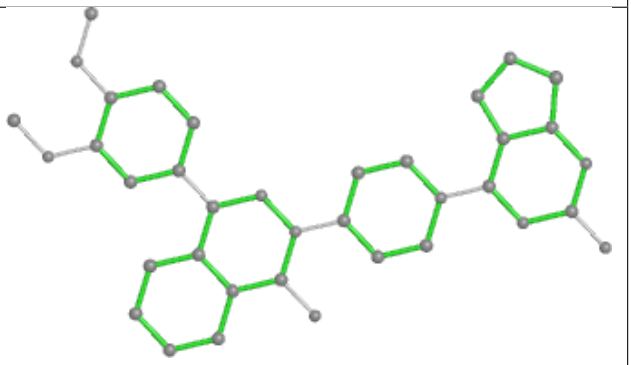
Bond lengths



Bond angles

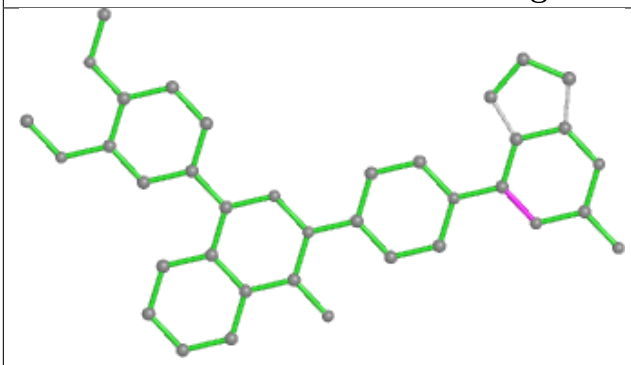


Torsions

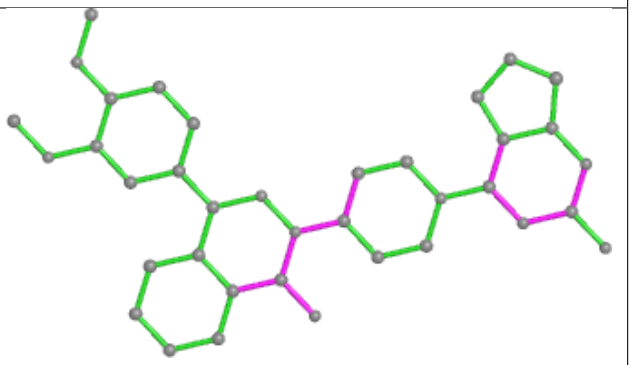


Rings

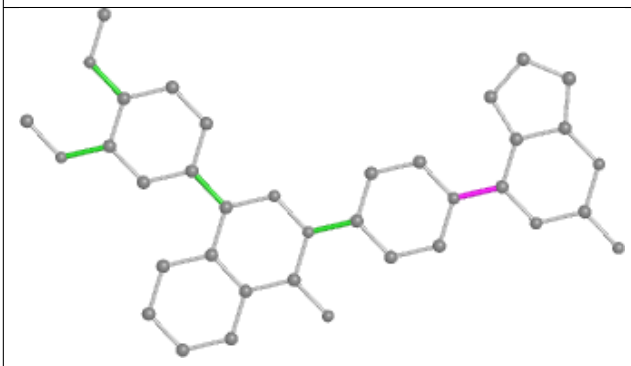
Ligand D62 B 516



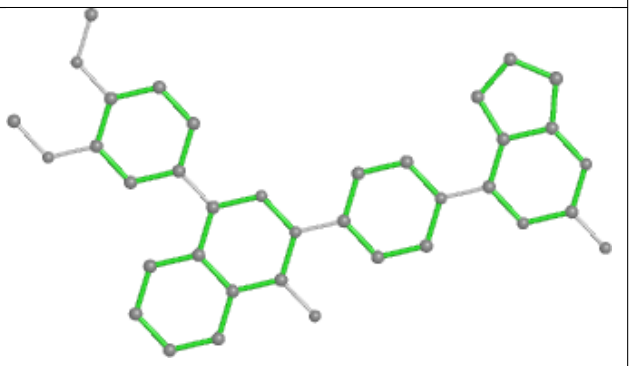
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	330/364 (90%)	0.38	30 (9%) 9 8	24, 37, 67, 98	0
1	B	323/364 (88%)	0.12	10 (3%) 49 48	25, 40, 60, 91	0
1	C	324/364 (89%)	0.21	18 (5%) 24 23	25, 40, 73, 92	0
1	D	324/364 (89%)	-0.09	6 (1%) 66 65	23, 31, 54, 83	0
All	All	1301/1456 (89%)	0.16	64 (4%) 29 28	23, 37, 65, 98	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	SER	6.1
1	A	411	PRO	5.8
1	A	362	ASN	5.3
1	A	410	ILE	4.8
1	C	363	ALA	4.6
1	A	353	GLU	4.5
1	C	294	SER	4.4
1	A	375	TYR	4.3
1	C	411	PRO	4.2
1	A	363	ALA	4.1
1	C	362	ASN	3.9
1	C	375	TYR	3.8
1	A	361	HIS	3.7
1	A	82	PHE	3.7
1	A	293	THR	3.6
1	C	361	HIS	3.5
1	B	91	VAL	3.5
1	C	356	PRO	3.4
1	D	362	ASN	3.4
1	A	295	SER	3.4
1	A	354	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	359	ASP	3.3
1	C	410	ILE	3.2
1	C	353	GLU	3.2
1	A	364	SER	3.0
1	A	234	LEU	3.0
1	C	293	THR	2.9
1	B	90	ASP	2.9
1	A	83	GLY	2.8
1	A	359	ASP	2.8
1	A	351	GLY	2.8
1	B	219	LEU	2.8
1	A	236	VAL	2.8
1	A	219	LEU	2.8
1	A	222	MET	2.7
1	B	221	LEU	2.7
1	C	354	ILE	2.6
1	A	235	ALA	2.6
1	B	222	MET	2.6
1	C	219	LEU	2.5
1	C	221	LEU	2.5
1	A	349	GLU	2.5
1	D	236	VAL	2.5
1	D	363	ALA	2.3
1	A	348	ARG	2.3
1	D	89	GLU	2.3
1	C	351	GLY	2.3
1	B	228	VAL	2.3
1	A	365	VAL	2.3
1	B	92	LEU	2.2
1	A	358	CYS	2.2
1	A	292	VAL	2.2
1	C	297	VAL	2.2
1	D	235	ALA	2.2
1	A	240	LEU	2.1
1	C	355	SER	2.1
1	B	362	ASN	2.1
1	B	223	TYR	2.1
1	B	229	LEU	2.1
1	C	235	ALA	2.1
1	D	354	ILE	2.1
1	A	199	ILE	2.0
1	A	202	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	291	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	C	512	4/4	0.63	0.58	63,68,70,75	0
4	EDO	A	525	4/4	0.69	0.35	58,64,64,70	0
5	PEG	C	519	7/7	0.71	0.24	43,57,66,75	0
5	PEG	D	518	7/7	0.75	0.19	50,56,60,68	0
8	PG4	C	502	13/13	0.76	0.33	46,73,84,85	0
4	EDO	B	514	4/4	0.76	0.21	57,62,69,69	0
5	PEG	D	509	7/7	0.78	0.29	44,55,69,75	0
5	PEG	A	511	7/7	0.79	0.28	44,68,77,80	0
4	EDO	D	522	4/4	0.79	0.21	39,40,45,48	0
4	EDO	A	509	4/4	0.79	0.23	66,67,72,76	0
5	PEG	A	519	7/7	0.80	0.16	58,64,71,73	0
4	EDO	D	506	4/4	0.80	0.24	51,52,53,61	0
5	PEG	D	508	7/7	0.81	0.18	43,60,69,72	0
8	PG4	C	521	13/13	0.81	0.28	38,46,59,65	0
4	EDO	B	517	4/4	0.82	0.37	66,69,75,79	0
4	EDO	D	513	4/4	0.82	0.23	43,45,47,55	0
4	EDO	B	505	4/4	0.82	0.23	54,58,63,63	0
4	EDO	C	503	4/4	0.83	0.83	73,78,78,84	0
5	PEG	A	510	7/7	0.84	0.19	55,71,76,78	0
5	PEG	A	518	7/7	0.84	0.38	59,63,70,71	0
4	EDO	B	510	4/4	0.84	0.62	54,57,62,62	0
4	EDO	B	504	4/4	0.84	0.30	70,75,77,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	508	4/4	0.85	0.31	60,69,69,80	0
4	EDO	C	501	4/4	0.85	0.48	48,48,60,66	0
4	EDO	D	515	4/4	0.86	0.25	53,65,68,76	0
4	EDO	B	518	4/4	0.86	0.35	48,54,57,67	0
4	EDO	C	516	4/4	0.86	0.16	43,47,50,52	0
4	EDO	C	515	4/4	0.86	0.25	58,66,70,70	0
5	PEG	B	508	7/7	0.86	0.40	49,67,72,80	0
4	EDO	D	520	4/4	0.87	0.20	64,65,68,74	0
6	D62	A	520	37/37	0.87	0.18	32,40,96,104	0
4	EDO	C	510	4/4	0.87	0.23	59,67,72,72	0
4	EDO	C	518	4/4	0.88	0.18	64,64,67,77	0
4	EDO	B	513	4/4	0.88	0.55	47,55,62,63	0
4	EDO	B	511	4/4	0.88	0.27	52,58,58,62	0
4	EDO	D	521	4/4	0.89	0.24	34,42,48,51	0
4	EDO	A	503	4/4	0.89	0.23	51,53,54,56	0
6	D62	C	520	37/37	0.90	0.15	33,39,100,107	0
5	PEG	A	516	7/7	0.90	0.20	39,59,73,75	0
4	EDO	A	521	4/4	0.90	0.14	54,65,68,78	0
4	EDO	C	508	4/4	0.90	0.16	57,58,63,66	0
4	EDO	A	522	4/4	0.90	0.47	49,56,64,69	0
4	EDO	B	515	4/4	0.90	0.20	50,54,61,65	0
4	EDO	A	523	4/4	0.90	0.23	51,56,56,58	0
4	EDO	B	512	4/4	0.90	0.16	60,62,67,80	0
4	EDO	A	514	4/4	0.91	0.13	49,50,55,57	0
5	PEG	C	513	7/7	0.91	0.12	53,58,64,68	0
4	EDO	B	520	4/4	0.91	0.19	50,52,59,65	0
4	EDO	C	511	4/4	0.91	0.14	52,56,60,61	0
4	EDO	B	507	4/4	0.91	0.22	52,55,61,62	0
5	PEG	D	510	7/7	0.91	0.21	56,69,80,92	0
4	EDO	B	519	4/4	0.91	0.28	63,63,68,70	0
4	EDO	A	504	4/4	0.91	0.27	53,65,67,78	0
4	EDO	D	501	4/4	0.91	0.13	51,53,53,54	0
4	EDO	C	517	4/4	0.91	0.11	66,67,71,76	0
4	EDO	C	509	4/4	0.92	0.25	54,55,59,59	0
4	EDO	C	504	4/4	0.92	0.17	51,56,56,60	0
4	EDO	A	515	4/4	0.92	0.28	36,48,53,53	0
7	EPE	B	521	15/15	0.93	0.23	52,77,92,93	0
4	EDO	C	507	4/4	0.93	0.19	52,52,63,63	0
6	D62	D	517	37/37	0.93	0.12	26,32,74,89	0
4	EDO	D	504	4/4	0.93	0.13	31,32,32,33	0
4	EDO	A	505	4/4	0.93	0.18	42,49,54,65	0
5	PEG	A	517	7/7	0.93	0.17	31,43,48,53	0

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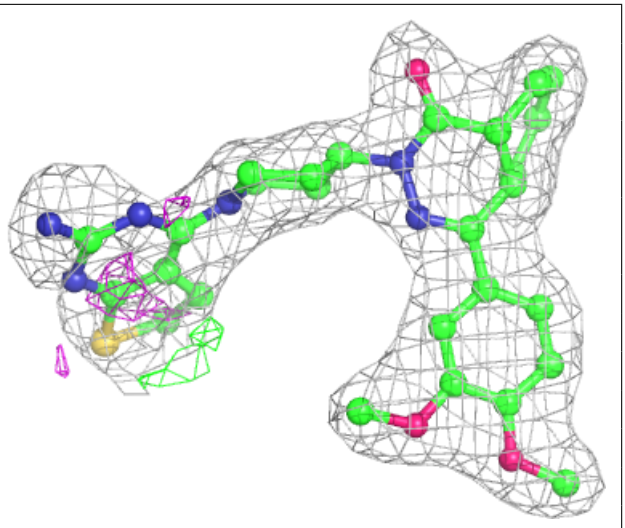
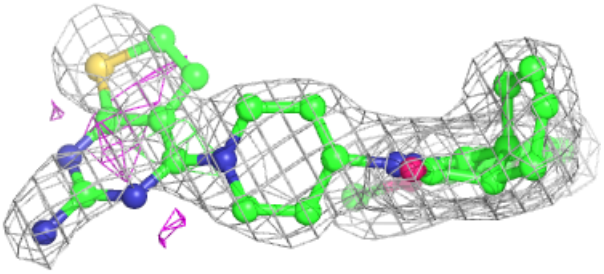
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	503	4/4	0.93	0.14	37,41,41,43	0
4	EDO	A	506	4/4	0.93	0.11	39,43,46,50	0
4	EDO	D	514	4/4	0.93	0.13	30,41,43,47	0
4	EDO	C	522	4/4	0.94	0.21	49,49,58,68	0
4	EDO	B	506	4/4	0.94	0.12	54,57,60,62	0
5	PEG	D	519	7/7	0.94	0.22	37,42,49,51	0
4	EDO	D	511	4/4	0.94	0.35	42,43,43,61	0
4	EDO	A	512	4/4	0.94	0.26	44,47,48,49	0
6	D62	B	516	37/37	0.94	0.12	27,33,74,78	0
4	EDO	D	505	4/4	0.95	0.09	41,43,43,48	0
4	EDO	A	513	4/4	0.95	0.21	45,51,53,64	0
4	EDO	A	507	4/4	0.95	0.15	50,61,65,67	0
4	EDO	D	507	4/4	0.95	0.16	38,50,52,55	0
4	EDO	D	516	4/4	0.95	0.14	37,39,45,47	0
7	EPE	B	509	15/15	0.96	0.14	53,62,70,73	0
7	EPE	A	524	15/15	0.96	0.23	44,77,92,96	0
2	ZN	A	501	1/1	0.97	0.07	33,33,33,33	0
4	EDO	D	512	4/4	0.97	0.07	38,41,43,46	0
7	EPE	D	523	15/15	0.97	0.14	36,72,91,103	0
7	EPE	C	514	15/15	0.98	0.15	40,46,80,101	0
3	MG	B	502	1/1	0.98	0.17	22,22,22,22	0
2	ZN	B	501	1/1	0.99	0.08	33,33,33,33	0
3	MG	A	502	1/1	0.99	0.15	19,19,19,19	0
3	MG	D	503	1/1	0.99	0.15	18,18,18,18	0
2	ZN	C	505	1/1	1.00	0.10	33,33,33,33	0
3	MG	C	506	1/1	1.00	0.17	21,21,21,21	0
2	ZN	D	502	1/1	1.00	0.11	30,30,30,30	0

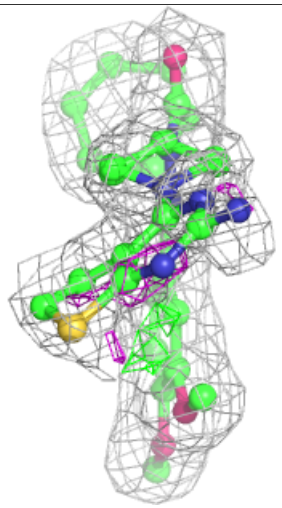
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around D62 A 520:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

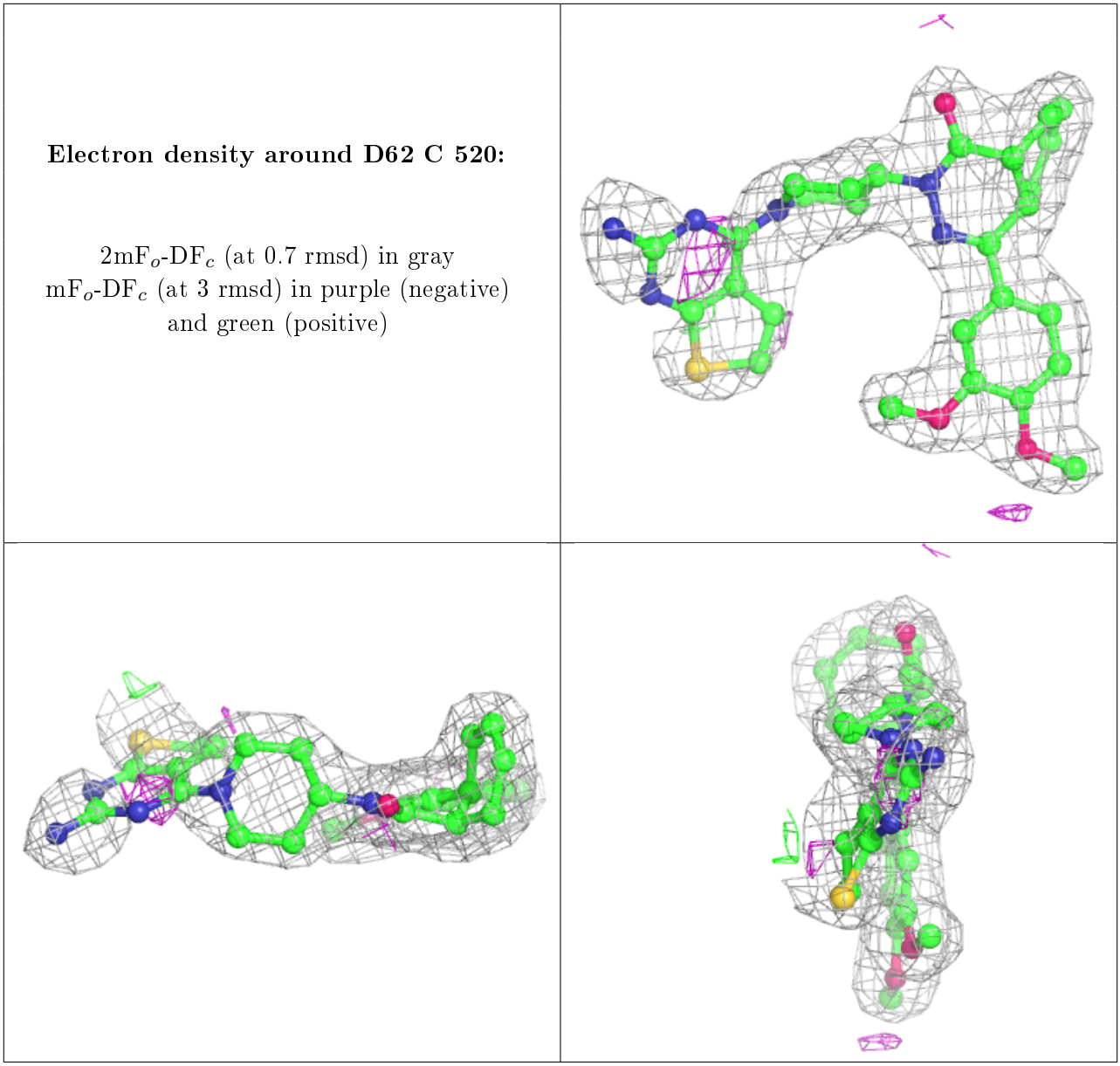






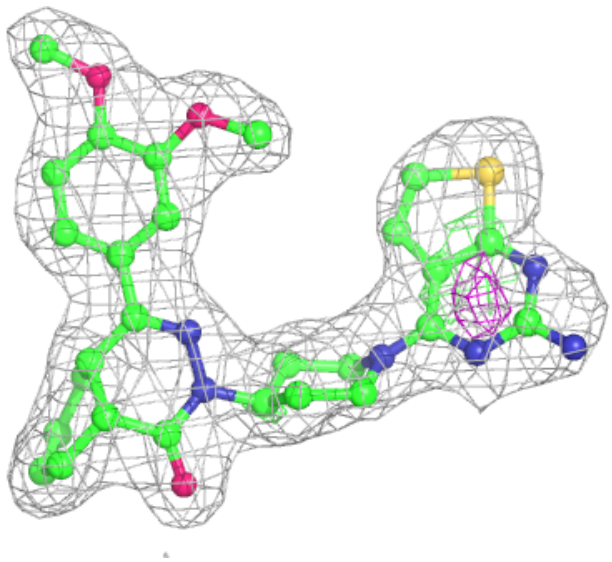
Electron density around D62 C 520:

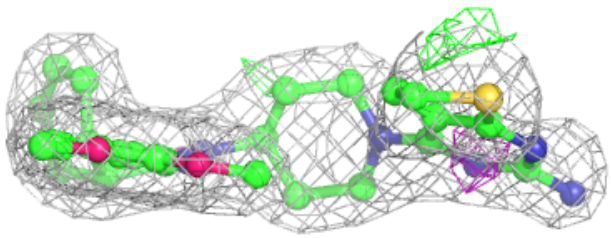
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

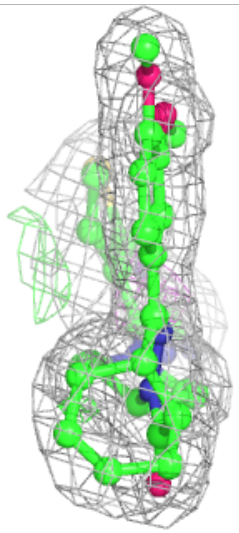


Electron density around D62 D 517:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

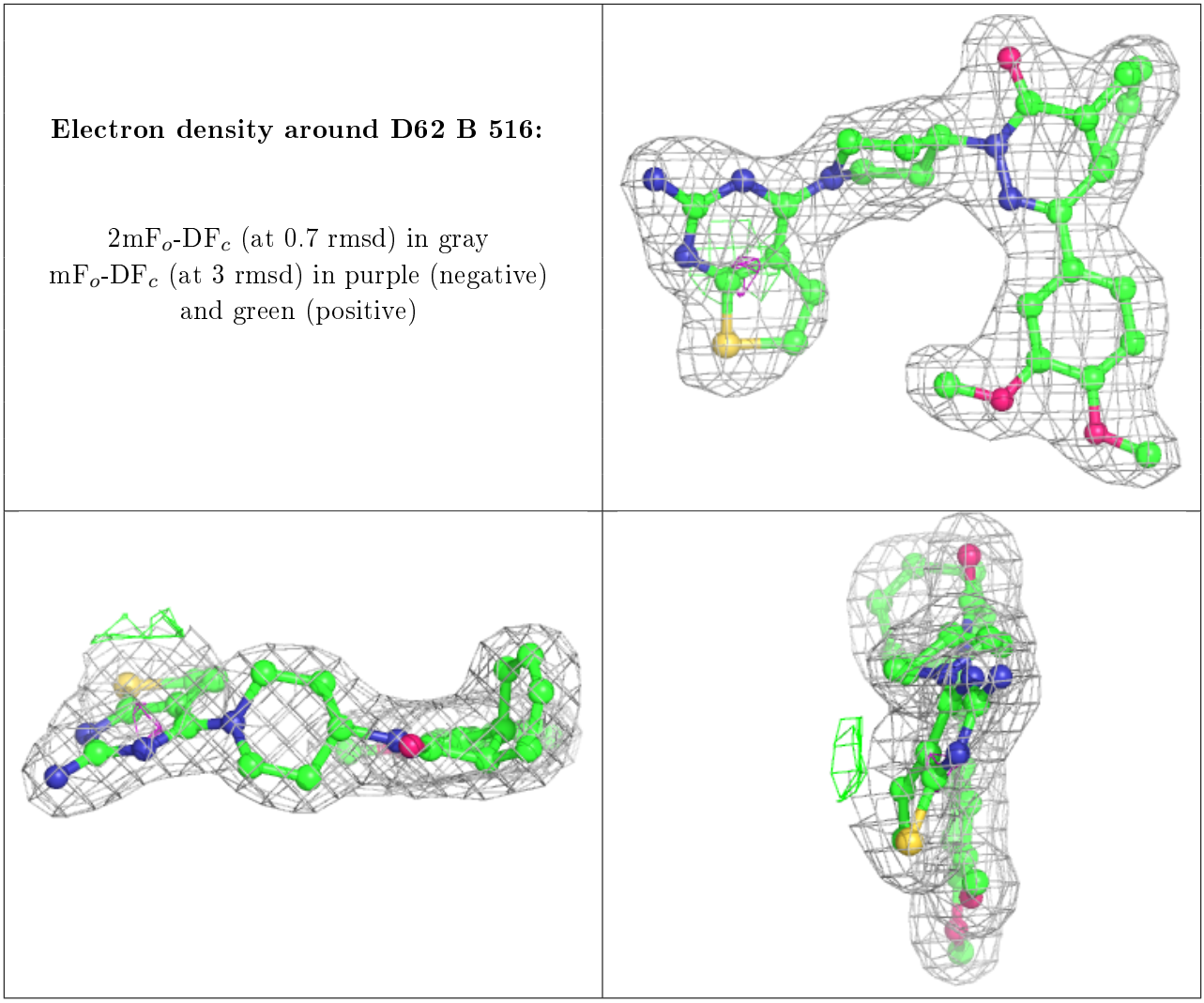






Electron density around D62 B 516:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.